Chapter 36
Partial phase shift and Green's function

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton

(Date: December 05, 2010)

36.1 Introduction

We now look for the solution of the Schrödinger equation for a particle in the presence of potential energy $V(r)$;

$$\psi_{klm} = R_{kl}(r) Y_l^m(\theta,\phi) = \frac{u_{kl}(r)}{r} Y_l^m(\theta,\phi)$$

with

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_{kl}}{dr}\right) + \left[k^2 - \frac{l(l+1)}{r^2} - U(r)\right]R_{kl} = 0$$

where

$$U(r) = \frac{2\mu}{\hbar^2} V(r)$$

and μ is a reduced mass. Note that $u_{kl}(r)$ satisfies the differential equation

$$\frac{d^2}{dr^2} u_{kl}(r) + \left[k^2 - \frac{l(l+1)}{r^2} - U(r)\right] u_{kl}(r) = 0$$

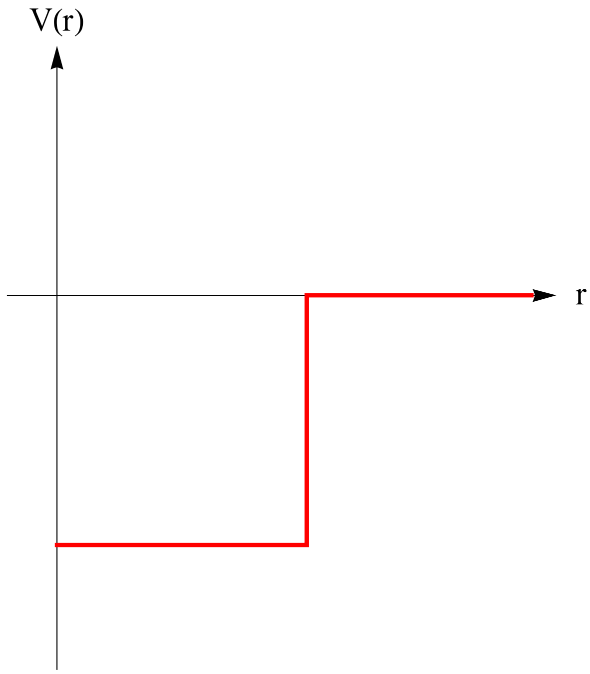
(i) Case-1

The radial equation for the external region $r>a$, where the scattering potential vanishes, is equal to

$$\frac{d^2}{dr^2} u_{kl}(r) + \left[k^2 - \frac{l(l+1)}{r^2}\right] u_{kl}(r) = 0 .$$

The solution of $R_{kl}(r)$ is

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \alpha_l j_l(kr) + \beta_l n_l(kr) \qquad \text{for } r>a.$$



(iii) Case-2

In the complete absence of a scattering potential ($V = 0$ everywhere),

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \gamma_l j_l(kr)$$

The condition of the normalization:

$$4\pi\gamma_l^2 \int_0^\infty drr^2[j_l(kr)]^2 = 1$$

36.2 Asymptotic form

Far from the interaction point, where the potential is negligible, the scattered wave function has the general form

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \alpha_l j_l(kr) + \beta_l n_l(kr)$$

since the position of the particle is far from the origin, where the function $n_l(kr)$ is poorly behaved. We use

$$\alpha_l = a_l \cos\delta_l, \qquad \beta_l = -a_l \sin\delta_l$$

Then we have

$$\begin{aligned} R_{kl}(r) &= a_l[\cos\delta_l\, j_l(kr) - \sin\delta_l n_l(kr)] \\ &= a_l \cos\delta_l [j_l(kr) - \tan\delta_l n_l(kr)] \end{aligned}$$

Note that $\delta_l = 0$ for free particle (the case-1). Since

$$j_l(kr) \to \frac{\sin(kr - \frac{l\pi}{2})}{kr}, \qquad n_l(kr) \to -\frac{\cos(kr - \frac{l\pi}{2})}{kr}$$

as $r \to \infty$, then we have

$$\begin{aligned} R_{kl}(r) &= \frac{a_l \cos\delta_l \sin(kr - \frac{l\pi}{2})}{kr} + \frac{a_l \cos\delta_l \cos(kr - \frac{l\pi}{2})}{kr} \\ &= a_l \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \end{aligned}$$

or

$$R_{kl}(r) = a_l \frac{e^{-\delta_l}[e^{i(kr - \frac{l\pi}{2} + 2\delta_l)} - e^{-i(kr - \frac{l\pi}{2})}]}{2ikr}$$

If the potential is spherically symmetric, the scattering amplitude $\psi^{(+)}(r,\theta)$ is a function of r and θ:

$$L_z\psi^{(+)} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\psi^{(+)} = 0,$$

($m = 0$), leading to the form

$$\psi^{(+)}(r,\theta) = \sum_l c_l R_{kl}(r) Y_l^{m=0}(\theta) = \sum_l c_l \sqrt{\frac{2l+1}{4\pi}} R_{kl}(r) P_l(\cos\theta)$$

where c_l is constant. Note that

$$Y_l^{m=0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta).$$

The complete solution of the scattering wave function is

$$\psi^{(+)}(r,\theta)=\sum_l a_l \frac{i^l(2l+1)\sin(kr-\frac{l\pi}{2}+\delta_l)}{kr}P_l(\cos\theta) \qquad (1)$$

36.3 Partial wave expansion of the scattering amplitude

On the other hand, $\psi^{(+)}(r,\theta)$ has the form

$$\psi^{(+)}(r,\theta)=\frac{1}{(2\pi)^{3/2}}[e^{ikz}+\frac{1}{r}e^{ikr}f(\theta)]$$

Note that

$$e^{ikz}=e^{ikr\cos\theta}\to\sum_l \frac{i^l(2l+1)\sin(kr-\frac{l\pi}{2})}{kr}P_l(\cos\theta), \qquad (2)$$

(Rayleigh's expansion)

or

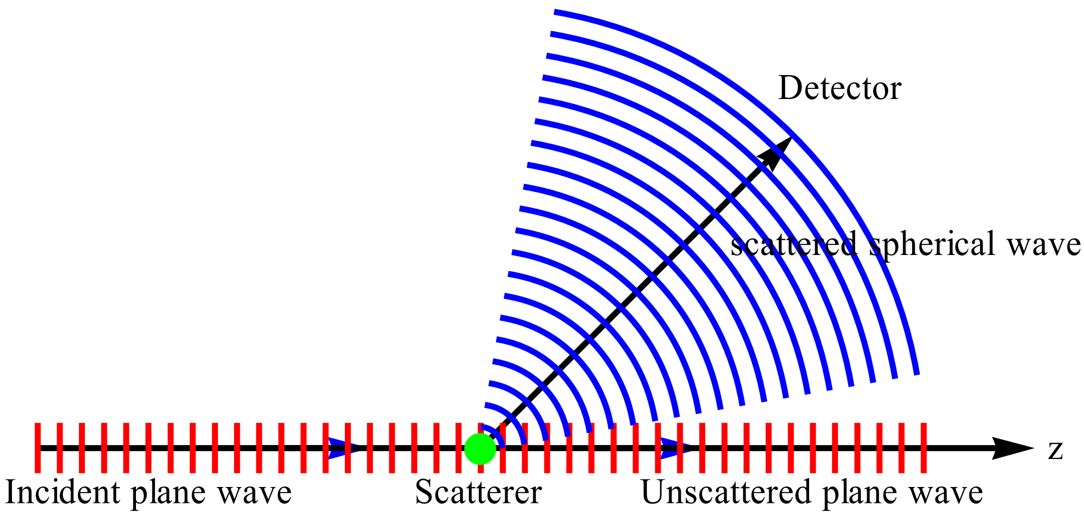
$$e^{ikz}\to\sum_l i^l\frac{2l+1}{2i}\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta).$$

From Eq.(1),

$$\psi^{(+)}(r,\theta)\to\sum_l a_l e^{-i\delta_l}i^l\left(\frac{2l+1}{2i}\right)\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2}+2\delta_l)}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta).$$

From Eq.(2),

$$\begin{aligned}\psi^{(+)}(r,\theta)&\approx e^{ikz}+\frac{1}{r}e^{ikr}f(\theta)\\&=\sum_l\left(\frac{2l+1}{2i}\right)i^l\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)+\frac{1}{r}e^{ikr}f(\theta)\end{aligned}$$



Therefore we have

$$\frac{1}{r}e^{ikr}f(\theta) = \sum_l a_l e^{-i\delta_l} i^l \left(\frac{2l+1}{2i}\right)\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2}+2\delta_l)} - e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

$$-\sum_l \left(\frac{2l+1}{2i}\right) i^l \frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

$$= \sum_l \{a_l e^{-i\delta_l} i^l \left(\frac{2l+1}{2i}\right)\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2}+2\delta_l)} - e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

$$-\sum_l \left(\frac{2l+1}{2i}\right) i^l \frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

The comparison leads to the condition for a_l.

$$-a_l e^{-i\delta_l} + 1 = 0, \qquad \text{or} \qquad a_l = e^{i\delta_l}.$$

Then

$$\frac{1}{r}e^{ikr}f(\theta) = \sum_l i^l \left(\frac{2l+1}{2i}\right)\frac{e^{ikr}}{kr}e^{i\delta_l}[e^{i(-\frac{l\pi}{2}+\delta_l)} - e^{i(-\frac{l\pi}{2}-\delta_l)}]P_l(\cos\theta)$$

Noting that

$$i^l = e^{i\frac{\pi l}{2}}$$

we have

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos\theta) ,$$

with

$$f_l(k) = \frac{1}{k} e^{i\delta_l} \sin(\delta_l) ,$$

or

$$kf_l(k) = e^{i\delta_l} \frac{1}{2i}[e^{i\delta_l} - e^{-i\delta_l}] = \frac{1}{2i}[e^{2i\delta_l} - 1] = \frac{i}{2}[1 - e^{2i\delta_l}] .$$

The total cross section is given by

$$\sigma_{tot} = \int |f(\theta)|^2 d\Omega$$

where

$$|f(\theta)|^2 = \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)(2l'+1) f_l^*(k) f_{l'}(k) P_l(\cos\theta) P_{l'}(\cos\theta)$$

Noting that

$$\int d\Omega P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1} \delta_{l,l'} ,$$

we have

$$\sigma_{tot} = 4\pi \sum_{l=0}^{\infty} (2l+1) |f_l(k)|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l .$$

36.4 Optical theorem

We can check the optical theorem

$$\mathrm{Im}[f(\theta = 0)] = \sum_{l=0}^{\infty} (2l+1) \mathrm{Im}[f_l(k)] P_l(\cos\theta) |_{\theta=0}$$

$$P_l(\cos\theta)|_{\theta=0} = 1$$

$$\mathrm{Im}[f_l(k)] = \frac{1}{k} \sin^2 \delta_l$$

$$\mathrm{Im}[f(\theta=0)] = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

Then we have

$$\sigma_{tot} = \frac{4\pi}{k}\mathrm{Im}[f(\theta=0)] \qquad \text{(optical theorem)}$$

We now consider the complex plane

$$z \equiv kf_l(k) = e^{i\delta_l}\sin(\delta_l) = \frac{1}{2i}[e^{2i\delta_l}-1] = \frac{i}{2}+\frac{1}{2}e^{i(2\delta_l-\frac{\pi}{2})}$$

or

$$z-\frac{i}{2} = \frac{1}{2}e^{i(2\delta_l-\frac{\pi}{2})}$$

This is a circle of radius ½ centered at (i/2).

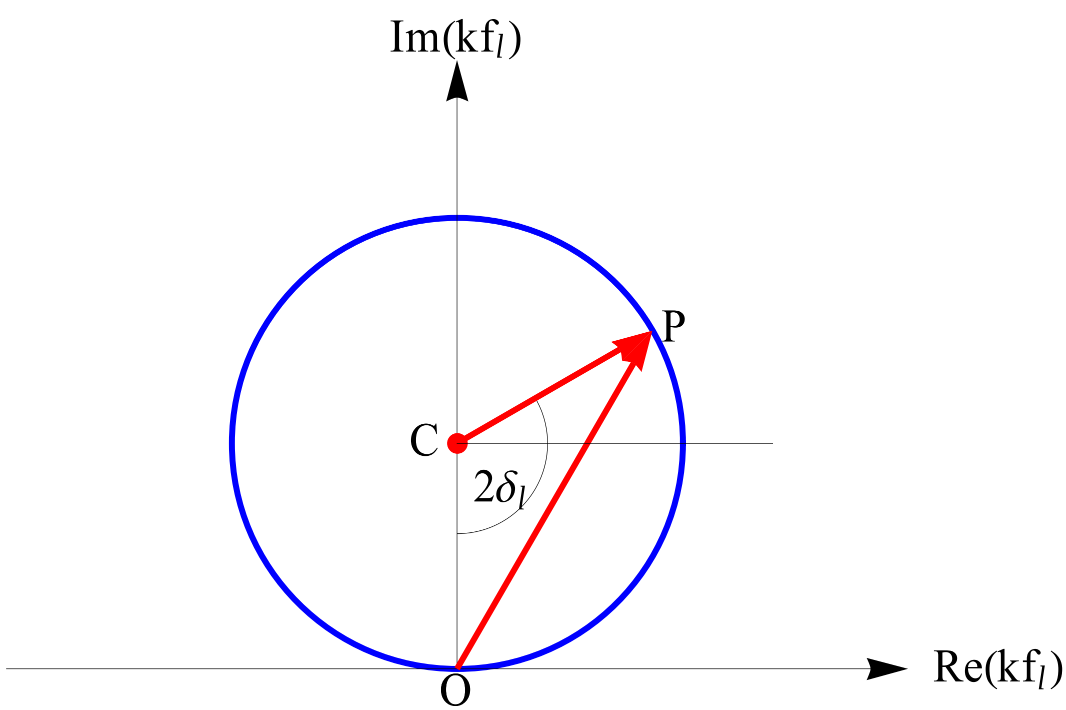


Fig. Argand diagram of $z = kf_l(k)$; The circle is called the unitary circle.

$OP = k|f_l(k)|$, $\overline{OC} = 1/2$, $\overline{CP} = 1/2$

$$\angle OCP = 2\delta_l$$

(i) $\delta_l \approx 0$

kf_l must stay near the bottom of the circle. kf_l may be positive or negative, but kf_l is almost purely real.

$$kf_l(k) = e^{i\delta_l}\sin(\delta_l) \approx \delta_l .$$

(ii) $\delta_l \approx \pi/2$

kf_l is almost purely imaginary and kf_l is maximal. Under such a condition the *l*-th partial wave may be in resonance.

$$kf_l(k) = e^{i\frac{\pi}{2}} = i .$$

$$\sigma_{tot}^{(l)} = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}(2l+1).$$

36.5 Comment: relative magnitude of phase shift

Classical mechanics:

$$L = ps .$$

Quantum mechanics:

$$L = \hbar\sqrt{l(l+1)} \approx \hbar l , \qquad p = \hbar k$$

r_0: the potential of interaction is appreciable only over the range r_0. If $s > r_0$, the interaction is negligible,

$$\frac{l}{p} = s > r_0$$

or

$$\frac{\hbar l}{\hbar k} > r_0 \qquad \text{or} \qquad l > r_0 k$$

The partial waves with **l** values in excess of $r_0 k$ will suffer little or no shift in phase.

36.8 Phase shift and Green's function

We use the following formula,

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = 4\pi ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi'), \qquad (1)$$

$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\, j_l(kr), \qquad (2)$$

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}}\sum_l C_l(2l+1)i^l R_{kl}{}^{(+)}(r)P_l(\cos\theta), \qquad (3)$$

and

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}}e^{ikz} - \int d^3\mathbf{r}'\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}U(r')\psi^{(+)}(r',\theta'), \qquad (4)$$

where

$$U(r) = \frac{2\mu}{\hbar^2}V(r).$$

Using the above relations, we can derive the integral equation for $R_{kl}(r)$.

$$C_l R_{kl}{}^{(+)}(r)P_l(\cos\theta) = j_l(kr)P_l(\cos\theta)$$
$$-ikC_l\sum_{l'}\sum_{m'=-l'}^{l'}\int_0^{\infty} r'^2\,dr' j_{l'}(kr_<)h_{l'}^{(1)}(kr_>)U(r')R_{kl}{}^{(+)}(r')Y_{l'}^{m'}(\theta,\phi)\int_0^{\pi}\sin\theta' d\theta'\int_0^{2\pi}d\phi' Y_{l'}^{m'^*}(\theta',\phi')P_l(\cos\theta')$$

Here we note that

$$\int_0^\pi \sin\theta' d\theta' \int_0^{2\pi} d\phi' Y_{l'}^{m'^*}(\theta',\phi') P_l(\cos\theta') = 2\pi\delta_{m',0} \int_0^\pi \sin\theta' d\theta' Y_{l'}^{0^*}(\cos\theta') P_l(\cos\theta')$$
$$= 2\pi\delta_{m',0} \sqrt{\frac{2l'+1}{4\pi}} \int_0^\pi \sin\theta' d\theta' P_{l'}(\cos\theta') P_l(\cos\theta')$$
$$= 2\pi\delta_{m',0} \sqrt{\frac{2l'+1}{4\pi}} \frac{1}{2l'+1} 2\delta_{l,l'}$$
$$= \sqrt{\frac{4\pi}{2l'+1}} \delta_{l,l'} \delta_{m',0}$$
$$= \sqrt{\frac{4\pi}{2l+1}} \delta_{l,l'} \delta_{m',0}$$

where

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta),$$

$$\int_0^\pi \sin\theta d\theta P_{l'}(\cos\theta) P_l(\cos\theta) = \frac{2}{2l+1}\delta_{l,l'}.$$

Then we have

$$C_l R_{kl}^{(+)}(r) P_l(\cos\theta) = j_l(kr) P_l(\cos\theta)$$
$$-ikC_l \sum_{l'} \sum_{m'=-l'}^{l'} \delta_{l,l'}\delta_{m',0} \int_0^\infty r'^2 dr' j_{l'}(kr_<) h_{l'}^{(1)}(kr_>) U(r') R_{kl}^{(+)}(r') \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \sqrt{\frac{4\pi}{2l+1}}$$

or

$$C_l R_{kl}^{(+)}(r) P_l(\cos\theta) = j_l(kr) P_l(\cos\theta)$$
$$-ikC_l \int_0^\infty r'^2 dr' j_l(kr_<) h_l^{(1)}(kr_>) U(r') R_{kl}^{(+)}(r') P_l(\cos\theta)$$

or

$$C_l R_{kl}^{(+)}(r) = j_l(kr)$$
$$-ikC_l \int_0^\infty r'^2 dr' j_l(kr_<) h_l^{(1)}(kr_>) U(r') R_{kl}^{(+)}(r')$$

or

$$C_l R_{kl}^{(+)}(r) = j_l(kr) - ikC_l h_l^{(1)}(kr)\int_0^r r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r')$$

$$-ikC_l \int_r^\infty r'^2\, dr' j_l(kr) h_l^{(1)}(kr')U(r')R_{kl}^{(+)}(r')$$

or

$$C_l R_{kl}^{(+)}(r) = j_l(kr) - ikC_l [j_l(kr) + in_l(kr)]\int_0^r r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r')$$

$$-ikC_l j_l(kr)\int_r^\infty r'^2\, dr'[j_l(kr') + in_l(kr')]U(r')R_{kl}^{(+)}(r')$$

since

$$h_l^{(1)}(kr) = j_l(kr) + in_l(kr).$$

Then we have

$$C_l R_{kl}^{(+)}(r) = j_l(kr)[1 - ikC_l \int_0^r r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r')] + kC_l \int_0^r r'^2\, dr' j_l(kr') n_l(kr)U(r')R_{kl}^{(+)}(r')$$

$$-ikC_l j_l(kr)\int_r^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r') + kC_l \int_r^\infty r'^2\, dr'\, j_l(kr) n_l(kr')]U(r')R_{kl}^{(+)}(r')$$

or

$$C_l R_{kl}^{(+)}(r) = j_l(kr)[1 - ikC_l \int_0^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r')]$$

$$+kC_l \int_0^\infty r'^2\, dr' j_l(kr_<) n_l(kr_>)U(r')R_{kl}^{(+)}(r')$$

Here we choose C_l such that

$$C_l = 1 - ikC_l \int_0^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}^{(+)}(r')]$$

or

$$C_l = \frac{1}{1 + ik\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')]}$$

Then we get

$$R_{kl}^{(+)}(r) = j_l(kr) + k\int_0^\infty r'^2\,dr' j_l(kr_<)n_l(kr_>)U(r')R_{kl}^{(+)}(r')$$

36.9 Physical meaning of C_l and δ_l

We consider $R_{kl}^{(+)}(r)$ for $r>a$, where $U(r) = 0$.

$$R_{kl}^{(+)}(r > a) = j_l(kr) + kn_l(kr)\int_0^r r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r') + kj_l(kr)\int_r^\infty r'^2\,dr' n_l(kr')U(r')R_{kl}^{(+)}(r')$$

$$= j_l(kr) + kn_l(kr)\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')$$

If we choose

$$\tan\delta_l = -k\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r'), \qquad (5)$$

then we get

$$R_{kl}^{(+)}(r > a) = j_l(kr) - \tan\delta_l n_l(kr)$$
$$= \frac{1}{\cos\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l n_l(kr)] \qquad (6)$$

$$C_l = \frac{1}{1 + ik\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')]}$$
$$= \frac{1}{1 - i\tan\delta_l} = e^{i\delta_l}\cos\delta_l$$

The wave function given by Eq.(3) has the form

$$\psi^{(+)}(r,\theta)=\frac{1}{(2\pi)^{3/2}}\sum_l e^{i\delta_l}(2l+1)i^l[\cos\delta_l j_l(kr)-\sin\delta_l n_l(kr)](r)P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_l e^{i\delta_l}(2l+1)i^l[\left(\frac{e^{i\delta_l}+e^{-i\delta_l}}{2}\right)j_l(kr)-\left(\frac{e^{i\delta_l}-e^{-i\delta_l}}{2i}\right)n_l(kr)](r)P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_l (\frac{2l+1}{2})i^l[e^{2i\delta_l}h_l^{(1)}(kr)+h_l^{(2)}(kr)](r)P_l(\cos\theta)$$

In the large limit of r, this solution is approximated by

$$\psi^{(+)}(r,\theta)=\frac{1}{(2\pi)^{3/2}}\sum_l (\frac{2l+1}{kr})i^l e^{i\delta_l}\sin(kr-\frac{l\pi}{2}+\delta_l)P_l(\cos\theta)$$

36.10 Determination of the phase shift.

In the first Born approximation,

$$R_{kl}^{(+)}(r)\approx j_l(kr)$$

Then we have

$$\tan\delta_l^{(1)}\approx -k\int_0^\infty r'^2\,dr'[j_l(kr')]^2U(r')$$

This approximation is good when the phase shift is small. The function $j_l(kr)$ is approximated by

$$j_l(x)\approx\frac{2^l\, l!}{(2l+1)!}(x)^l\,.$$

Then we have

$$\tan\delta_l^{(1)}\approx -\frac{2^l(l!)^2}{[(2l+1)!]^2}k^{2l+1}\int_0^\infty r'^{2l+2}\,dr'U(r')\,.$$

For low energies and high angular momenta,

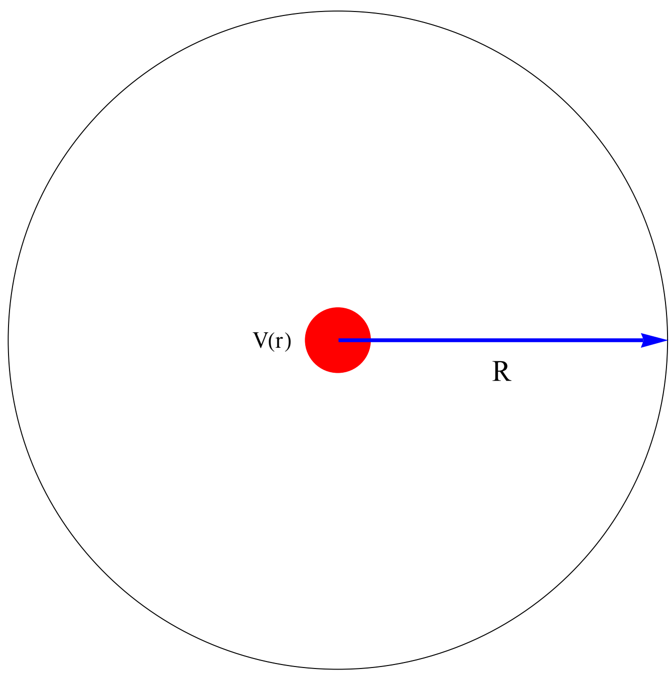
$$\delta_l^{(1)}\propto k^{2l+1}\,.$$

36.11 Friedel's sum rule (sold state physics)

Jacques Friedel, (February 11, 1921 à Paris, est un physicien français et professeur émérite à l'Université Paris-Sud Orsay.

http://fr.wikipedia.org/wiki/Jacques_Friedel

We consider a metal with a single impurity at zero temperature. Electrons are scattered by the impurity potential, and the charge distribution of electrons below the Fermi level changes. The Friedel's sum rule states that the "excess charge" due to a single impurity potential in a metal is equal to a sum of phase shifts for scatterings of electrons by the impurity. For simplicity, we consider a free electron gas and a spherical scattering potential $V(r)$.



Suppose that there is an impurity atom located at the origin. The total number of electrons inside the sphere with radius R is evaluated as

$$N_e = 2\int_0^R 4\pi r^2 dr \int_0^{k_F} 2\pi k^2 dk \int_0^\pi \sin\theta d\theta \left|\psi^{(+)}\right|^2$$
$$= 2\int_0^R 2\pi r^2 dr \int_0^{k_F} 4\pi k^2 dk \frac{2}{(2\pi)^3}\sum_l (\frac{2l+1}{k^2})\frac{[u_{kl}(r)]^2}{r^2}$$
$$= \frac{4}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \int_0^R [u_{kl}(r)]^2 dr$$

Here we note that

(i)

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}}\sum_l (\frac{2l+1}{k}) i^l e^{i\delta_l(k)} \frac{u_{kl}(r)}{r} P_l(\cos\theta)$$

with

$$u_{kl}(r) = \sin[kr - \frac{l\pi}{2} + \delta_l(k)]$$

$u_{kl}(r)$ satisfies the differential equation given by

$$\frac{d^2}{dr^2}u_{kl}(r) + [k^2 - \frac{l(l+1)}{r^2} - U(r)]u_{kl}(r) = 0\,.$$

(ii)

$$\int_0^\pi \sin\theta d\theta \left|\psi^{(+)}(r,\theta)\right|^2 = \frac{1}{(2\pi)^3}\sum_l\sum_{l'}(\frac{2l+1}{k^2})(2l'+1)\frac{[u_{kl}(r)]^2}{r^2}\int_0^\pi \sin\theta d\theta P_l(\cos\theta)P_{l'}(\cos\theta)$$
$$= \frac{1}{(2\pi)^3}\sum_l\sum_{l'}(\frac{2l+1}{k^2})(2l'+1)\frac{[u_{kl}(r)]^2}{r^2}\frac{2}{2l+1}\delta_{l,l'}$$
$$= \frac{2}{(2\pi)^3}\sum_l (\frac{2l+1}{k^2})\frac{[u_{kl}(r)]^2}{r^2}$$

where

$$\int_{-1}^1 P_l(\mu)P_{l'}(\mu)d\mu = \frac{2}{2l+1}\delta_{l,l'}\,. \qquad \text{(orthogonality)}$$

(iii)

From the two differential equations with k and k', we have

$$u_{kl}(r)\frac{d^2}{dr^2}u_{k'l}(r)+[k'^2-\frac{l(l+1)}{r^2}-U(r)]u_{kl}(r)u_{k'l}(r)=0$$

$$u_{k'l}(r)\frac{d^2}{dr^2}u_{kl}(r)+[k^2-\frac{l(l+1)}{r^2}-U(r)]u_{k'l}(r)u_{kl}(r)=0$$

The subtraction of these equations leads to

$$u_{kl}(r)\frac{d^2}{dr^2}u_{k'l}(r)-u_{k'l}(r)\frac{d^2}{dr^2}u_{kl}(r)+(k'^2-k^2)u_{kl}(r)u_{k'l}(r)=0\,.$$

Then

$$\begin{aligned}(k'^2-k^2)\int_0^R u_{kl}(r)u_{k'l}(r)dr &= \int_0^R [u_{k'l}(r)\frac{d^2}{dr^2}u_{kl}(r)-u_{kl}(r)\frac{d^2}{dr^2}u_{k'l}(r)]dr \\ &= [u_{k'l}(r)\frac{d}{dr}u_{kl}(r)-u_{kl}(r)\frac{d}{dr}u_{kl'}(r)]_0^R \\ &= [u_{k'l}(r)\frac{d}{dr}u_{kl}(r)-u_{kl}(r)\frac{d}{dr}u_{kl'}(r)]_{r=R}\end{aligned}$$

since $u_{kl}(r=0)=0$. In the limit of $k'\rightarrow k$, we have

$$2k\int_0^R [u_{kl}(r)]^2\,dr=[\frac{\partial u_{kl}(r)}{\partial k}\frac{du_{kl}(r)}{dr}-u_{kl}(r)\frac{\partial^2 u_{kl}(r)}{\partial k\partial r}]_{r=R}$$

(iv)
From (i), (ii), and (iii), we obtain

$$\int_0^R [u_{kl}(r)]^2\,dr=\frac{1}{2k}\{k(R+\frac{d\delta_l(k)}{dk})-\frac{1}{2}\sin[2(kR+\delta_l(k)-\frac{l\pi}{2}]\}$$

where

$$u_{kl}(r)=\sin[kr-\frac{l\pi}{2}+\delta_l(k)]$$

((Mathematica))

```
u[k_, l_, r_] = Sin[k r - (l π)/2 + δ[l, k]];

f1 =
 (D[u[k, l, r], k] D[u[k, l, r], r] -
     u[k, l, r] D[ D[u[k, l, r], k], r]) /. r → R //
  Simplify
```

$$k R + \frac{1}{2} \mathrm{Sin}[l \pi - 2 k R - 2 \delta[l, k]] + k \delta^{(0,1)}[l, k]$$

Thus the number of electrons inside the radius R is

$$N_e = \frac{4}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \frac{1}{2k}\{k(R + \frac{d\delta_l(k)}{dk}) - \frac{1}{2}\sin[2(kR + \delta_l(k) - \frac{l\pi}{2}]\}$$
$$= \frac{2}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \{(R + \frac{d\delta_l(k)}{dk}) - \frac{1}{2k}\sin[2(kR + \delta_l(k) - \frac{l\pi}{2}]\}$$

under the presence of the potential $V(r)$. In the absence of the potential, the number of electrons inside the radius R is evaluated as

$$N_e^{\,0} = \frac{2}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \{R - \frac{1}{2k}\sin[2(kR - \frac{l\pi}{2}]\}$$

since $\delta_l(k) = 0$ for the free particles. The difference in the number of electrons with and without the impurity is

$$\Delta N_e = N_e - N_e^{\,0}$$
$$= \frac{2}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \{\frac{d\delta_l(k)}{dk} - \frac{1}{2k}\sin[2(kR + \delta_l(k) - \frac{l\pi}{2}] + \frac{1}{2k}\sin[2(kR - \frac{l\pi}{2}]\}$$
$$= \frac{2}{\pi}\sum_l (2l+1)\int_0^{k_F} dk \{\frac{d\delta_l(k)}{dk} - \frac{1}{k}\sin\delta_l(k)\cos[2kR - l\pi + \delta_l(k)]\}$$

We assume that $\frac{1}{k}\sin\delta_l(k)$ is slowly varying function of k. Then we get

$$\Delta N_e = \frac{2}{\pi}\sum_l (2l+1)\{\delta_l(k_F) - \frac{1}{2k_F R}\sin\delta_l(k_F)\sin[2k_F R - l\pi + \delta_l(k_F)]\}$$
$$= \frac{2}{\pi}\sum_l (2l+1)\delta_l(k_F)$$

when $R \to \infty$. Here ($2l$+1) is the orbital degeneracy. The factor 2 is the spin degeneracy. In general, $\Delta N_e = Z$, where Z is the valency of the impurity relative to that of the host lattice. Then we have

$$Z = \frac{2}{\pi}\sum_l (2l+1)\delta_l(k_F). \qquad \text{(Friedel's sum rule)}$$

The total screening charge must equal the charge which it screens. The number Z is the valence difference between the impurity and the solvent metal, because we need precisely this number of extra electrons in the neighborhood of the impurity to neutralize its charge.

36.12 Resistivity

The reciporocal of the mean free time τ_i is expressed by

$$\frac{1}{\tau_i} = n_i \sigma_e v_F,$$

where n_i is the concentration of impurity and v_F is the Fermi velocity. σ_e is the scattering cross section and is given by

$$\sigma_e = 2\pi\int_0^\pi \sigma(\theta)(1-\cos\theta)\sin\theta d\theta$$

where $\sigma(\theta)$ is the cross section per unit solid angle for scattering of a conduction electron by an impurity atom.

$$\sigma(\theta) = |f(\theta)|^2 = |\sum_{l=0}^{\infty}(2l+1)\frac{1}{k}e^{i\delta_l}\sin(\delta_l)P_l(\cos\theta)|^2$$
$$= \frac{1}{k_F^2}|\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin(\delta_l)P_l(\cos\theta)|^2$$
$$= \frac{1}{k_F^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)e^{i\delta_l}e^{-i\delta_{l'}}\sin(\delta_l)\sin(\delta_{l'})P_l(\cos\theta)P_{l'}(\cos\theta)$$

We need to calculate I which is related to the effective average cross section for resistivity

$$
\begin{aligned}
I &= \int_0^{\pi} (1-\cos\theta)\sin\theta P_l(\cos\theta)P_{l'}(\cos\theta)d\theta \\
&= \int_{-1}^{1} (1-\mu)d\mu P_l(\mu)P_{l'}(\mu) \\
&= \int_{-1}^{1} d\mu P_l(\mu)P_{l'}(\mu) - \int_{-1}^{1} \mu d\mu P_l(\mu)P_{l'}(\mu) \\
&= \frac{2}{2l+1}(\delta_{l,l'} - \frac{l+1}{2l+3}\delta_{l',l+1} - \frac{l}{2l-1}\delta_{l',l-1})
\end{aligned}
$$

((Note))

$$
\int_{-1}^{1} \mu d\mu P_l(\mu)P_{l'}(\mu) = \frac{2(l+1)}{(2l+1)(2l+3)}\delta_{l',l+1} + \frac{2l}{(2l-1)(2l+1)}\delta_{l',l-1} \qquad \text{(Jackson, p.100)}
$$

Then we get

$$
\begin{aligned}
\sigma_e &= \frac{2\pi}{k_F{}^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)e^{i\delta_l}e^{-i\delta_{l'}}\sin(\delta_l)\sin(\delta_{l'})\int_{-1}^{1}(1-\mu)d\mu P_l(\mu)P_{l'}(\mu) \\
&= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}[e^{i\delta_l}e^{-i\delta_{l'}}\sin(\delta_l)\sin(\delta_{l'})(2l'+1)\{\delta_{l,l'} - \frac{l+1}{2l+3}\delta_{l',l+1} - \frac{l}{2l-1}\delta_{l',l-1}\}] \\
&= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}[l\sin^2(\delta_l) + (l+1)\sin^2(\delta_l) - (l+1)e^{i\delta_l}e^{-i\delta_{l+1}}\sin(\delta_l)\sin(\delta_{l+1}) - le^{i\delta_l}e^{-i\delta_{l-1}}\sin(\delta_l)\sin(\delta_{l-1})] \\
&= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}[(l+1)\sin^2(\delta_{l+1}) + (l+1)\sin^2(\delta_l) - (l+1)e^{i\delta_l}e^{-i\delta_{l+1}}\sin(\delta_l)\sin(\delta_{l+1}) \\
&\quad -(l+1)e^{i\delta_{l+1}}e^{-i\delta_l}\sin(\delta_{l+1})\sin(\delta_l)]
\end{aligned}
$$

or

$$
\begin{aligned}
\sigma_e &= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}(l+1)[\sin^2(\delta_{l+1}) + \sin^2(\delta_l) - e^{i\delta_l}e^{-i\delta_{l+1}}\sin(\delta_l)\sin(\delta_{l+1}) - e^{i\delta_{l+1}}e^{-i\delta_l}\sin(\delta_{l+1})\sin(\delta_l)] \\
&= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}(l+1)[\sin^2(\delta_{l+1}) + \sin^2(\delta_l) - 2\sin(\delta_l)\sin(\delta_{l+1})\cos(\delta_l - \delta_{l+1})] \\
&= \frac{4\pi}{k_F{}^2}\sum_{l=0}^{\infty}(l+1)\sin^2(\delta_l - \delta_{l+1})
\end{aligned}
$$

((Mathematica))

```
f1 =
 Sin[δ[l]]^2 + Sin[δ[l + 1]]^2 -
    2 Sin[δ[l]] Sin[δ[l + 1]]
     Cos[δ[l] - δ[l + 1]] // TrigFactor //
  FullSimplify

Sin[δ[l] - δ[1 + l]]^2
```

The contribution ρ_i of the scattering centers to the electrical resistivity is

$$\rho_i = \frac{m}{ne^2} n_i \sigma_e v_F = \frac{4\pi\hbar n_i}{ne^2 k_F} \sum_{l=0}^{\infty} (l+1)\sin^2(\delta_l - \delta_{l+1})$$

Here the phase shift are to be taken at the Fermi surface.

36.13 Example

In the Friedel's sum rule, we assume that only one phase shift is large.

$$Z = \frac{2}{\pi}(2L+1)\delta_L(k_F),$$

or

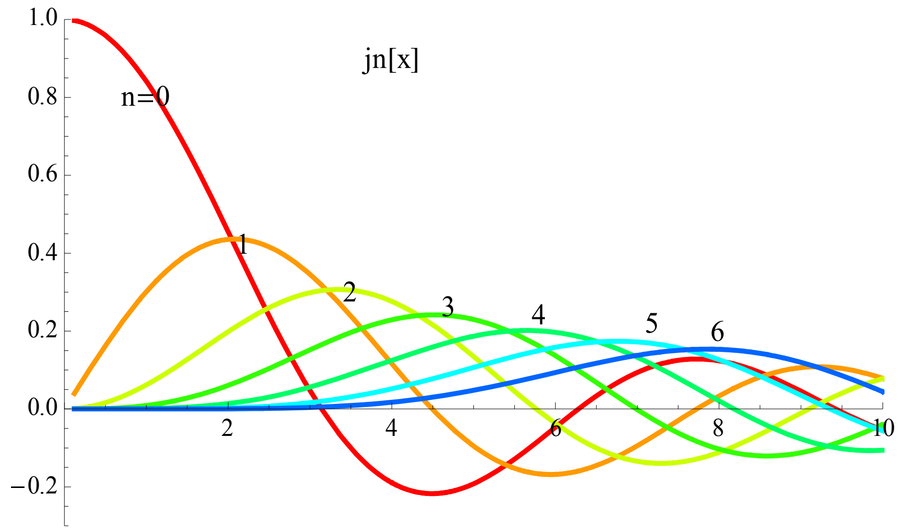
$$\delta_L(k_F) = \frac{\pi Z}{2(2L+1)}.$$

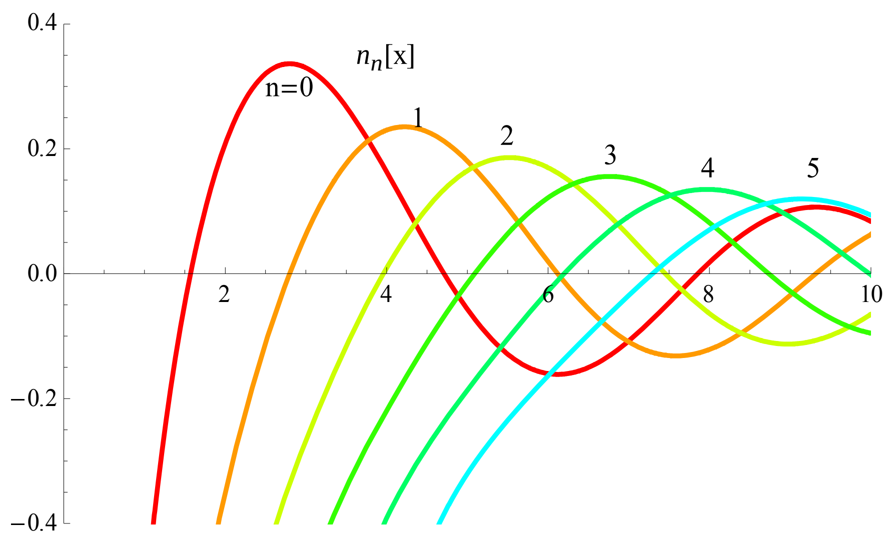
Then the resistivity is evaluated as

$$\begin{aligned}\rho_i &= \frac{m}{ne^2} n_i \sigma_e v_F \\ &= \frac{4\pi\hbar n_i}{ne^2 k_F}[(L+1)\sin^2(\delta_L(k_F)) + L\sin^2(\delta_L(k_F))] \\ &= \frac{4\pi\hbar n_i}{ne^2 k_F}(2L+1)\sin^2(\delta_L(k_F)) = \frac{4\pi\hbar n_i}{ne^2 k_F}(2L+1)\sin^2(\frac{\pi Z}{4L+2})\end{aligned}$$

APPENDIX

((**Mathematica**))
Spherical Bessel function, spherical Neuman function, spherical Hankel function





REFERENCES

Merzbacher, *Quantum Mechanics*, 3rd edition (John-Wiley & Sons, New York, 1998).
S. Sunagawa, *Quantum theory of scattering* (Iwanami, Tokyo, 1977).
C. Kittel, *Quantum Theory of Solids*, 2nd edition (John Wiley & Sons, Inc., New York, 1963).
J.M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960). p.226.
J.M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, 1964).
K. Yosida, Theory of Magnetism (Springer Verlag, Berlin, 1996).
J. Kondo, The Physics of Dilute Magnetic Alloys, 6-th edition (Syokabo, Tokyo, 1994) [in Japanese].